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Application of response surface methodology and artificial neural network methods in modelling and optimization of biosorption process

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HIGHLIGHTS

- Theoretical background of optimization methods (RSM and ANN).
- Design of experiments as a tool for improving efficiency of the processes.
- Optimization of biosorption process using response surface methodology (RSM).
- Optimization of biosorption process using artificial neural networks (ANN).

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ABSTRACT

A review on the application of response surface methodology (RSM) and artificial neural networks (ANN) in biosorption modelling and optimization is presented. The theoretical background of the discussed methods with the application procedure is explained. The paper describes most frequently used experimental designs, concerning their limitations and typical applications. The paper also presents ways to determine the accuracy and the significance of model fitting for both methodologies described herein. Furthermore, recent references on biosorption modelling and optimization with the use of RSM and the ANN approach are shown. Special attention was paid to the selection of factors and responses, as well as to statistical analysis of the modelling results.

1. Introduction

Biosorption is a complex process (Witek-Krowiak and Reddy, 2013; Chojnacka, 2010) dependent on many factors whose total effect has a direct impact on the process performance. Therefore it is important to select an appropriate mathematical model for predicting and optimizing the system. The optimization and modelling of biosorption is still in the stage of research. Commonly used models employed to describe equilibrium and kinetic studies, for instance the Langmuir (Chojnacka, 2007), Freundlich (Witek-Krowiak et al., 2011) or pseudo-second-order models (Witek-Krowiak, 2012), may be found insufficient in determining the connection between the factors and evaluating their impact on the biosorption process.

Optimization is a method for determining the best solution in terms of certain quality criteria (such as process efficiency) and leads to improving the performance of the designed system or process. The optimization of the biosorption process aims at finding the specific conditions (environmental and/or design parameters) at which the process would give the best possible response (best efficiency or uptake). Usually experiments are carried out in such a way that one factor is being applied and analyzed whereas the others remain unaffected. This procedure is called *one variable at time* (OVAT). A method is time consuming (the researcher has to screen all variables independently) and requires a large number of experiments, which leads to high costs of study. Additionally, OVAT does not include the interactions between the selected parameters.

Multivariate statistics techniques allow a significant reduction in the number of experiments, and the description of the impact of the independent variables (individually or in combination) in the process (Amini et al., 2009). This contributes to the development and optimization of the operating system, significantly decreasing the cost of experiments. *Response surface methodology* (RSM) and the *artificial neural network* (ANN) are among the most popularly used methods in research on biosorption literature. RSM and ANN provide an alternative for systems where the mathematical relationship between the parameters and the responses is unknown. Both are powerful data modelling tools, which are able to capture and represent complex nonlinear relationships between independent variables and responses of the system.

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1.1. Response surface methodology (RSM)

Response surface methodology is a set of mathematical techniques that describe the relation between several independent variables and one or more responses. This method was developed by Box and Wilson (1951) and since then it has been widely used as a technique for designing experiments. The RSM method is based on the fit of mathematical models (linear, square polynomial functions and others) to the experimental results generated from the designed experiment and the verification of the model obtained by means of statistical techniques. The design of experiment (DOE) is a fundamental tool in the field of engineering. This technique can be used especially for improving efficiency of the processes. The basic idea of DOE is to diversify all significant parameters simultaneously over a set of designed experiments and then to combine the results through a mathematical model. Afterwards, this model can be gradually used for optimization, predictions or interpretation. This leads to improving process performance, reducing the number of variables in the process by taking into account only most significant factors, and also to reducing operation costs and experimental time (Montgomery and Runger, 2003; Ghorbani et al., 2008).

The optimization by means of RSM approach could be divided into six stages (Fig. 1): (1) selection of independent variables and possible responses, (2) selection of experimental design strategy, (3) execution of experiments and obtaining results, (4) fitting the model equation to experimental data, (5) obtaining response graphs and verification of the model (ANOVA), (6) determination of optimal conditions.

1.1.1. Selection of independent variables and possible response

The first and most important step in the whole procedure is to select the most important variables and their ranges from the collection of possible candidates. The batch biosorption process is usually influenced by several environmental factors (Table 1), like pH, temperature, solute and sorbent concentration, time of the process, agitation speed. If biosorption is carried out in the column mode, important variables include bed height, liquid velocity and particles diameter. Sometimes researchers have searched for optimal condition for biosorbent preparation, selecting reaction conditions as crucial factors (Ahmad and Alrozi, 2010; Mao et al., 2011). Among a multitude of parameters it is important to select the most important, whose effect on the process is most significant. For this purpose, screening experiments should be applied. As an example, the Plackett–Burman (PB) design, two-level full or fractional factorial designs give an opportunity to identify those variables that have a major effect on the output data. An another type of experimental design used for the selection of the significant factors is the Minimum Run Equireplicated Resolution V Design (Cao et al., 2010). The biggest advantage of this design is that it combines great reduction of required experiments and high resolution. Which means, that it takes into consideration 2 and 3-level interactions. In the next stage the determination of the levels of the parameters should be made. A properly selected range of variables increases the chance of response optimum identification.

1.1.2. Selection of experimental design strategy

The next crucial step is the design of an experiment with the selection of the points where the response should be estimated. Several design methods have been applied for biosorption optimization, the most popular being the central composite design (CCD), Box–Behnken design (BB), Doehlert Matrix (D), as well as Plackett–Burman (PB) design, full or fractional factorial designs for optimizations with many variables (Fig. 2). Researchers can easily get access to the software that provides simple and clear use of these methods. The most popular programs for biosorption studies are Design Expert (Stat-Ease, Inc.), Minitab (Minitab Inc.), Statistica (StatSoft), JMP (SAS) and Matlab (MathWorks).

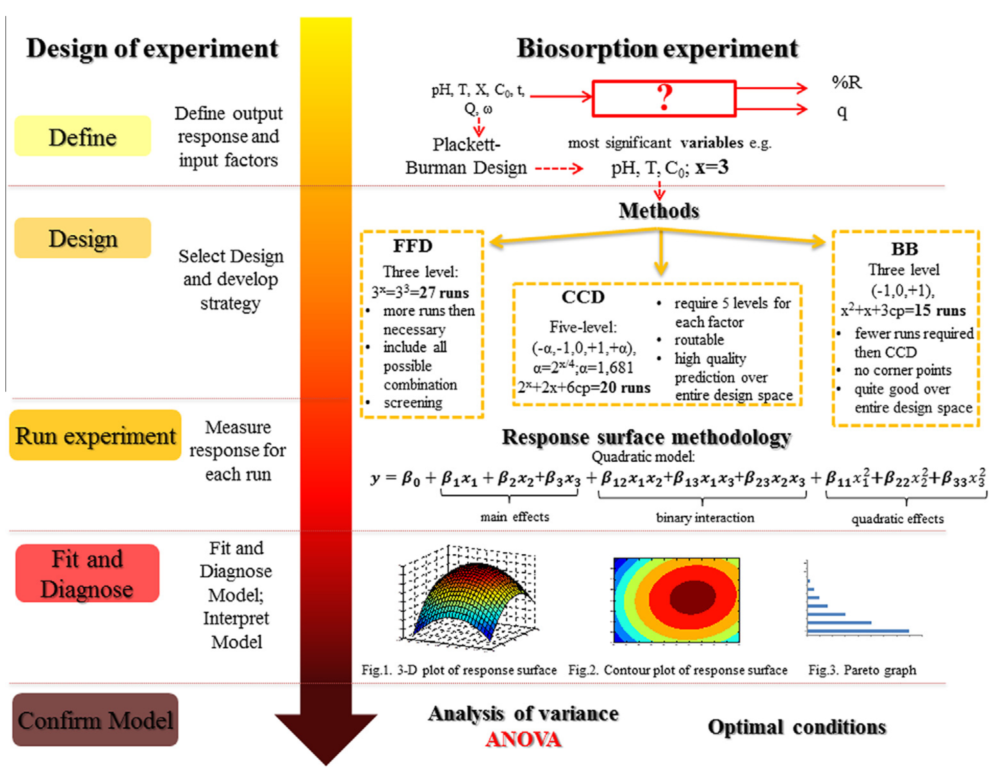

Fig. 1. Design of experiment in RSM methodology.